

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 May 12 EXTEND option available in structure searching
NEWS 4 May 12 Polymer links for the POLYLINK command completed in REGISTRY
NEWS 5 May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAPLUS
NEWS 6 May 27 CAPLUS super roles and document types searchable in REGISTRY
NEWS 7 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
NEWS 8 Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
NEWS 9 Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 10 Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS 11 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 12 AUG 02 CAPLUS and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 13 AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS 14 AUG 02 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 15 AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:54:43 ON 09 AUG 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 09 AUG 2004

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Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 7 AUG 2004 HIGHEST RN 723734-66-5
 DICTIONARY FILE UPDATES: 7 AUG 2004 HIGHEST RN 723734-66-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

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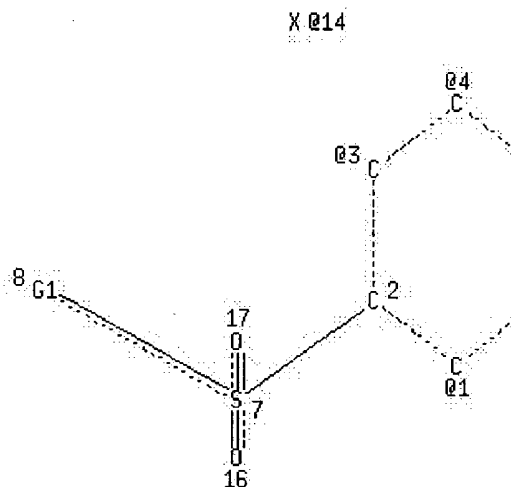
L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

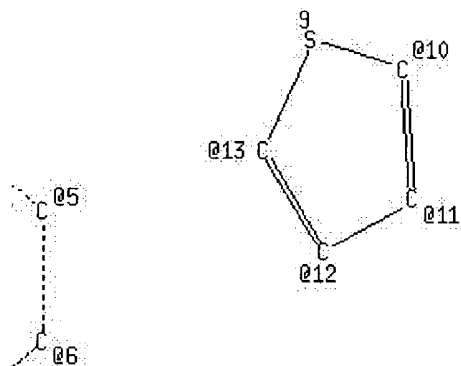
L1 STR

AK199M2



Page 1-A

C4 @15



Page 1-B

VAR G1=18/19

VPA 14-1/3/4/5/6 S

VPA 15-10/11/12/13 S

NODE ATTRIBUTES:

HCOUNT	IS M2	AT	19
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 14 16 17 18 19

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 10:57:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1647 TO ITERATE

60.7% PROCESSED 1000 ITERATIONS

2 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 30506 TO 35374

h eb c g cg b cg

eb

PROJECTED ANSWERS: 2 TO 173

L2 2 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 10:57:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 32122 TO ITERATE

100.0% PROCESSED 32122 ITERATIONS

41 ANSWERS

SEARCH TIME: 00.00.01

L3 41 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

156.68

156.89

FILE 'HCAPLUS' ENTERED AT 10:57:16 ON 09 AUG 2004

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FILE COVERS 1907 - 9 Aug 2004 VOL 141 ISS 7

FILE LAST UPDATED: 8 Aug 2004 (20040808/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 14 L3

=> s 14 and brown, d?/au

7837 BROWN, D?/AU

L5 2 L4 AND BROWN, D?/AU

=> d 15, ibib abs fhitr, 1-2

L5 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text  CAS

ACCESSION NUMBER: 2001:798214 HCAPLUS

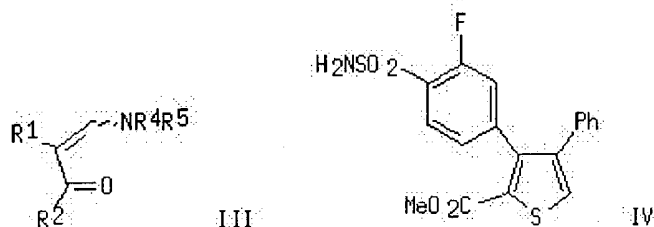
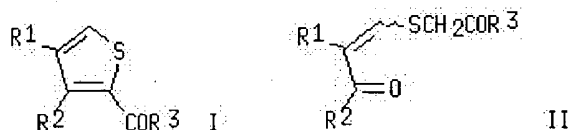
DOCUMENT NUMBER: 135:344368

TITLE: Process for the regioselective synthesis of 3,4-diaryl substituted thiophenes

INVENTOR(S): Brown, David L.; Ludwig, Cindy L.

PATENT ASSIGNEE(S): Pharmacia Corporation, USA
 SOURCE: PCT Int. Appl., 74 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081333	A2	20011101	WO 2001-US13092	20010420
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002183362	A1	20021205	US 2001-839424	20010420
EP 1276736	A2	20030122	EP 2001-928781	20010420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 6600052	B1	20030729	US 2001-838986	20010420
JP 2003531202	T2	20031021	JP 2001-578424	20010420
US 2003232996	A1	20031218	US 2003-258507	20030416
<u>PRIORITY APPLN. INFO.:</u>			US 2000-199533P	P 20000425
			US 2000-253380P	P 20001127
			WO 2001-US13092	W 20010420
OTHER SOURCE(S):			CASREACT 135:344368; MARPAT 135:344368	
GI				



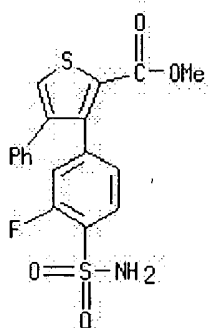
AB A novel process for the regioselective prepn. of I, via the intermediates II and III using an alkali metal alkoxide ring cyclizing reagent where (R1 and R2 = substituted carbocycle or heterocycle; R3 = OR6 or NR7R8 and R6, R7 and R8 = H, (un)heterosubstituted hydrocarbonyl; R4 and R5 are independently H and optionally substituted alkyl), was accomplished. Thus IV was prepd. in 66 % yield via the enamine intermediate of Me 3-[3-fluoro-4-(methylthio)phenyl]-4-phenyl-2-thiophenecarboxylate.

IT 370874-59-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of 3,4-diarylthiophene)

RN 370874-59-2 HCAPLUS

CN 2-Thiophenecarboxylic acid, 3-[4-(aminosulfonyl)-3-fluorophenyl]-4-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

References

ACCESSION NUMBER: 2001:798213 HCAPLUS
DOCUMENT NUMBER: 135:344477
TITLE: Preparation of 2-fluorobenzenesulfonyl-heterocycles with COX-1 and COX-2 inhibiting activity for pharmaceutical use in the treatment of inflammation
INVENTOR(S): Brown, David L.; Graneto, Matthew J.; Ludwig, Cindy L.; Talley, John J.
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 242 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081332	A2	20011101	WO 2001-US12983	20010420
WO 2001081332	A3	20020404		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002183362	A1	20021205	US 2001-839424	20010420
EP 1296971	A2	20030402	EP 2001-927279	20010420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 6600052	B1	20030729	US 2001-838986	20010420
JP 2003531201	T2	20031021	JP 2001-578423	20010420
US 2004092552	A1	20040513	US 2003-258493	20030711
PRIORITY APPLN. INFO.:			US 2000-199533P	P 20000425
			US 2000-253380P	P 20001127
			WO 2001-US12983	W 20010420

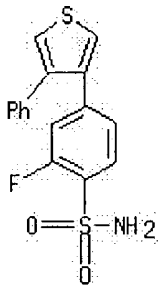
OTHER SOURCE(S): MARPAT 135:344477
GI



IT 370874-28-5P

(prepn. of 2-fluorobenzenesulfonyl-heterocycles with COX-1 and COX-2 inhibiting activity for pharmaceutical use in the treatment of inflammation)

CN Benzenesulfonamide, 2-fluoro-4-(4-phenyl-3-thienyl)- (9CI) (CA INDEX NAME)



(FILE 'HOME' ENTERED AT 10:54:43 ON 09 AUG 2004)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 09 AUG 2004

L2	2	S	L1	
L3	41	S	L1	FULL

FILE 'HCAPLUS' ENTERED AT 10:57:16 ON 09 AUG 2004

L4 14 S L3
L5 2 S L4 AND BROWN, D?/AU

$\Rightarrow s$ 14 not 15

h eb c g cg b cg

eb'

L6 12 L4 NOT L5

=> s l6 and graneto, m?/au
40 GRANETO, M?/AU

L7 0 L6 AND GRANETO, M?/AU

=> s l6 and ludwig, c?/au
270 LUDWIG, C?/AU

L8 0 L6 AND LUDWIG, C?/AU

=> d l6, ibib abs fhitstr, 1-12

L6 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text CATE References

ACCESSION NUMBER: 2004:565073 HCAPLUS
TITLE: Use of cathepsin k inhibitors for the treatment of glaucoma
INVENTOR(S): Shepard, Allan; Clark, Abbot F.; Jacobson, Nasreen
PATENT ASSIGNEE(S): Alcon, Inc., Switz.
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058238	A1	20040715	WO 2003-US40511	20031219
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2002-436126P P 20021223
AB Compns. contg. inhibitors of cathepsin K (CTSK) expression and/or activity are provided. Methods for the treatment of glaucoma using the compns. of the invention are further provided. The cathepsin K antagonist is selected from, but not limited to, the group consisting of monensin, brefeldin A, tunicamycin and 1,3-bis(acylamino)-2-propanone derivs., cycloalttilisin 6, cycloalttilisin 7, AC-3-1, AC-3-3, AC-5-1, haploscleridamine, SB-331750, SB-357114, peptidomimetic aminomethyl ketones, α, α' -diacylamino ketones, alkoxymethyl ketones, cyanamides, pyridoxal propionate derivs. (including Clik-164 and Clik-166), SB-290190, α -alkoxy ketone derivs., cyanamide derivs., and N α -acyl- α -amino acid-(arylaminoethyl)amides.

IT 190658-17-4

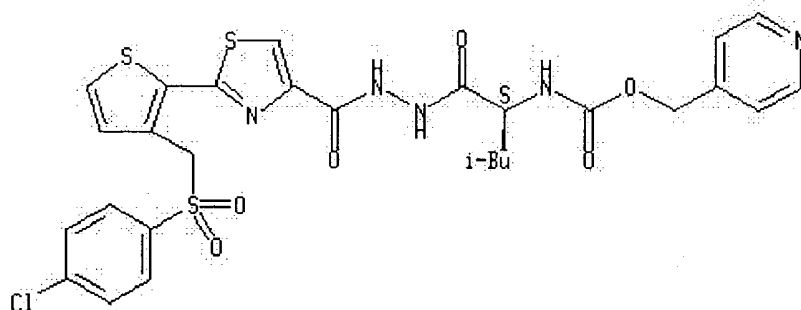
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of cathepsin k inhibitors for treatment of glaucoma)

RN 190658-17-4 HCAPLUS

CN 4-Thiazolecarboxylic acid, 2-[3-[(4-chlorophenyl)sulfonyl]methyl]-2-

thienyl]-, 2-[(2S)-4-methyl-1-oxo-2-[[[(4-pyridinylmethoxy)carbonyl]amino]p
entyl]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

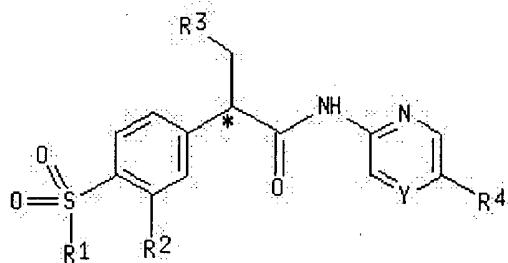
Full
Text

Chemical
References

ACCESSION NUMBER: 2004:515493 HCAPLUS
DOCUMENT NUMBER: 141:71565
TITLE: Preparation of pyrazines and related compounds as glucokinase activators for the treatment of type II diabetes
INVENTOR(S): Chen, Shaoqing; Corbett, Wendy Lea; Guertin, Kevin Richard; Haynes, Nancy-Ellen; Kester, Robert Francis; Mennona, Francis A.; Mischke, Steven Gregory; Qian, Yimin; Sarabu, Ramakanth; Scott, Nathan Robert; Thakkar, Kshitij Chhabilbhai
PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.
SOURCE: PCT Int. Appl., 243 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052869	A1	20040624	WO 2003-EP14055	20031211
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004147748	A1	20040729	US 2003-732838	20031210
PRIORITY APPLN. INFO.:			US 2002-432806P	P 20021212
			US 2003-524531P	P 20031124

GI



I

AB Title compd. I [R1 = alkyl; R2 = H, halo, nitro, etc.; R3 = cycloalkyl; R4 = SO₂NR₅R₆, NHSO₂CH₃, [CH₂]_mNMe₂, etc.; R5 = H, alkyl; R6 = alkyl; Y = CH, N; * denotes an asym. carbon] and their pharmaceutically acceptable salts were prepd. For example, the Pd-catalyzed coupling of 2-amino-5-bromopyrazine with NaSMe, followed by reaction with (2R)-(3-chloro-4-metnanesufonylphenyl)-3-cyclopentylpropionic acid afforded compd. (R)-I [R1 = Me; R2 = Cl; R3 = cyclopetyl; R4 = SMe; Y = N] in 22.1% overall yield. In glucokinase activity assays (in vitro) using glucose-6-phosphate dehydrogenase (G6PDH), compds. I exhibited SC_{1.5} values less than or equal to 100 μM. Formulations are given. Compds. I are claimed useful for the treatment and prophylaxis of II type diabetes.

IT **710321-98-5P**

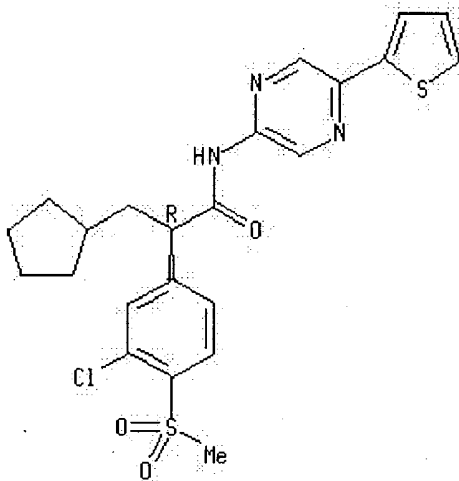
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazines and related compds. as glucokinase activators for the treatment of type II diabetes)

RN **710321-98-5** HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



L6 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Chemical
References

ACCESSION NUMBER:

2002:145039 HCAPLUS

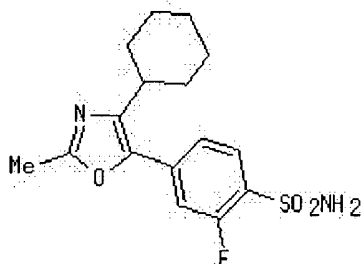
DOCUMENT NUMBER:

136:325469

TITLE:

4-(4-Cycloalkyl/aryl-oxazol-5-yl)benzenesulfonamides as Selective Cyclooxygenase-2 Inhibitors: Enhancement of the Selectivity by Introduction of a Fluorine Atom and Identification of a Potent, Highly Selective, and

Orally Active COX-2 Inhibitor JTE-522
 AUTHOR(S): Hashimoto, Hiromasa; Imamura, Katsuaki; Haruta, Jun-ichi; Wakitani, Korekiyo
 CORPORATE SOURCE: Central Pharmaceutical Research Institute, JT Inc., Takatsuki, Osaka, 569-1125, Japan
 SOURCE: Journal of Medicinal Chemistry (2002), 45(7), 1511-1517
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A series of 4-(4-cycloalkyl/aryl-oxazol-5-yl)benzenesulfonamide derivs., e.g., I, were synthesized and evaluated for their abilities to inhibit cyclooxygenase-2 (COX-2) and cyclooxygenase-1 (COX-1) enzymes. In this series, substituent effects at the ortho position to the sulfonamide group on the Ph ring were examd. Most substituents reduced or lost both COX-2 and COX-1 activities. In contrast, introduction of a fluorine atom preserved COX-2 potency and notably increased COX1/COX-2 selectivity. This work led to the identification of a potent, highly selective, and orally active COX-2 inhibitor I (JTE-522), which is currently in phase II clin. trials for the treatment of rheumatoid arthritis, osteoarthritis, and acute pain.

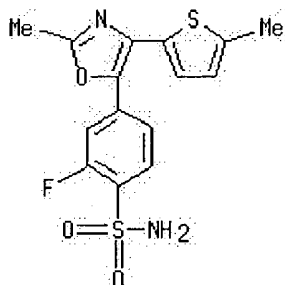
IT 415679-14-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of substituted benzenesulfonamides as selective cyclooxygenase-2 inhibitors from substituted benzyl bromides via coupling with acid chloride, conversion to α -acetoxy ketones, cyclocondensation to form oxazoles and sulfonamidation)

RN 415679-14-0 HCAPLUS

CN Benzenesulfonamide, 2-fluoro-4-[2-methyl-4-(5-methyl-2-thienyl)-5-oxazolyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
--------------	------------------------

ACCESSION NUMBER: 2002:72091 HCAPLUS
DOCUMENT NUMBER: 136:134566
TITLE: Synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compounds as β 3-adrenergic agonists
INVENTOR(S): Evers, Britta; Jesudason, Cynthia Darshini; Karanjawala, Rushad Eruch; Remick, David Michael; Ruehter, Gerd; Sall, Daniel Jon; Schotten, Theo; Siegel, Miles Goodman; Stenzel, Wolfgang; Stucky, Russell Dean; Werner, John Arnold
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2002006276</u>	A1	20020124	<u>WO 2001-US16519</u>	20010709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>AU 2001072917</u>	A5	20020130	<u>AU 2001-72917</u>	20010709
<u>EP 1303509</u>	A1	20030423	<u>EP 2001-952125</u>	20010709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
<u>BR 2001012409</u>	A	20030722	<u>BR 2001-12409</u>	20010709
<u>JP 2004504320</u>	T2	20040212	<u>JP 2002-512179</u>	20010709
<u>US 2003191156</u>	A1	20031009	<u>US 2002-311112</u>	20021213
<u>US 6730792</u>	B2	20040504		
<u>NO 2003000098</u>	A	20030109	<u>NO 2003-98</u>	20030109
<u>HR 2003000018</u>	A1	20030430	<u>HR 2003-18</u>	20030113
PRIORITY APPLN. INFO.:			<u>US 2000-217965P</u>	P 20000713
			<u>US 2000-241614P</u>	P 20001019
			<u>US 2001-292988P</u>	P 20010523
			<u>WO 2001-US16519</u>	W 20010709
OTHER SOURCE(S):	MARPAT 136:134566			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A1-3 = C, N provided that only one of A1-3 can be nitrogen; Het = (un)substituted, optionally benzofused 5 or 6 membered heterocyclic ring; R1,1a,1b = H, halo, OH, alkyl, alkoxy, haloalkyl, SO2-alkyl; R2 = H, alkyl; R3 = H alkyl; R4 = H, alkyl; or R3 and R4

combine with the carbon to which both are attached to form a C3-C6 cyclic ring; or R4 and X1 combine with the carbon to which both are attached to form a C3-C8 cyclic ring; or R4 combines with X1, the carbon to which both are attached, and the Ph group to which X1 is attached to form a benzofused cycloalkyl radical; X is OCH₂, SCH₂, bond; X1 = bond, divalent hydrocarbon moiety; X2 = O, S, NH, NHSO₂, SO₂NH, CH₂, bond; X3 = (un)substituted Ph, 5 or 6 membered heterocyclic ring] were prepd. For instance, 2-(1-methylpyrazol-3-yl)phenol was reacted with (2S)-glycidyl 3-nitrobenzenesulfonate (THF, t-BuOK, reflux, 16 h) to give epoxide II. This was reacted with the amine derived from 4-(2-amino-2-methylpropyl)phenol and 2-chloro-3-cyanopyridine (alc. solvent, 80°C, 2-72 h) to give III. The intrinsic activity (E_{max}) of representative compds. of the invention was assessed relative to isoproterenol (a nonselective β₃-agonist); III had E_{max} = 55.0%. I are used in the treatment of diabetes, obesity, etc.

IT 391922-26-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as β₃-adrenergic agonists)

RN 391922-26-2 HCAPLUS

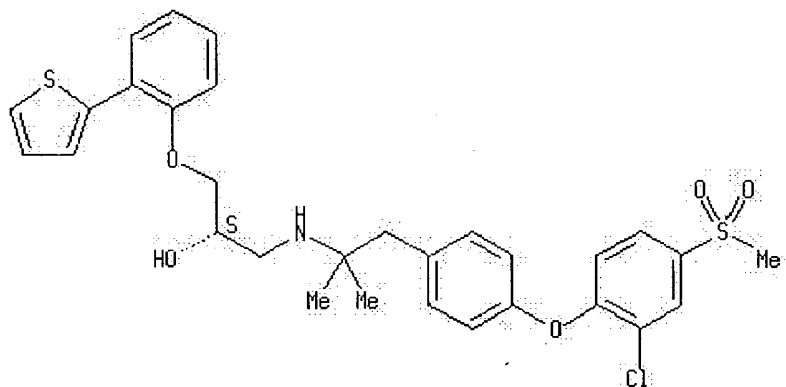
CN 2-Propanol, 1-[[[2-[4-[2-chloro-4-(methylsulfonyl)phenoxy]phenyl]-1,1-dimethylethyl]amino]-3-[2-(2-thienyl)phenoxy]-, (2S)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 391922-25-1

CMF C30 H32 Cl N O5 S2

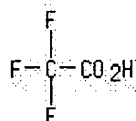
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2000:637744 HCAPLUS
 DOCUMENT NUMBER: 134:39080
 TITLE: A method for including protein flexibility in protein-ligand docking: improving tools for database mining and virtual screening
 AUTHOR(S): Broughton, H. B.
 CORPORATE SOURCE: Merck, Sharp & Dohme Neuroscience Research Centre, Essex, UK
 SOURCE: Journal of Molecular Graphics & Modelling (2000), 18(3), 247-257
 CODEN: JMGMF1; ISSN: 1093-3263
 PUBLISHER: Elsevier Science Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Second-generation methods for docking ligands into their biol. receptors, such as FLOG, provide for flexibility of the ligand but not of the receptor. Mol. dynamics based methods, such as free energy perturbation, account for flexibility, solvent effects, etc., but are very time consuming. We combined the use of statistical anal. of conformational samples from short-run protein mol. dynamics with grid-based docking protocols and demonstrated improved performance in two test cases. Our statistical anal. explores the importance of the av. strength of a potential interaction with the biol. target and optionally applies a weighting depending on the variability in the strength of the interaction seen during dynamics simulation. Using these methods, we improved the no. of known dihydrofolate reductase ligands found in the top-ranked 10% of a database of drug-like mols., in searches based on the three-dimensional structure of the protein. These methods are able to match the ability of manual docking to assess likely inactivity on steric grounds and indeed to rank order ligands from a homologous series of cyclooxygenase-2 inhibitors with good correlation to their true activity. Furthermore, these methods reduce the need for human intervention in setting up mol. docking expts.

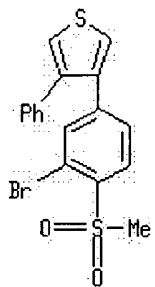
IT 312611-71-5

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(method for including protein flexibility in protein-ligand docking - improving tools for database mining and virtual screening)

RN 312611-71-5 HCAPLUS

CN Thiophene, 3-[3-bromo-4-(methylsulfonyl)phenyl]-4-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

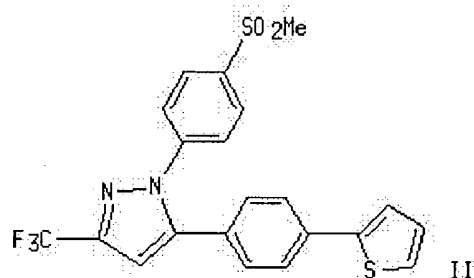
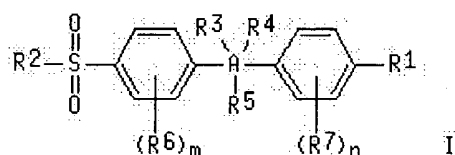
L6 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Links References
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ACCESSION NUMBER: 1999:795808 HCAPLUS
 DOCUMENT NUMBER: 132:35714
 TITLE: Preparation of heterocyclyl sulfonylbenzene compounds
 as anti-inflammatory/analgesic agents.
 INVENTOR(S): Ando, Kazuo; Kato, Tomoki; Kawai, Akiyoshi; Nonomura,
 Tomomi
 PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 236 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9964415</u>	A1	19991216	<u>WO 1999-IB970</u>	19990531
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>AU 9938414</u>	A1	19991230	<u>AU 1999-38414</u>	19990531
<u>EP 1086097</u>	A1	20010328	<u>EP 1999-921043</u>	19990531
<u>EP 1086097</u>	B1	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
<u>JP 2002517496</u>	T2	20020618	<u>JP 2000-553424</u>	19990531
<u>AT 267196</u>	E	20040615	<u>AT 1999-921043</u>	19990531
<u>ZA 9903897</u>	A	20010104	<u>ZA 1999-3897</u>	19990610
<u>US 6294558</u>	B1	20010925	<u>US 1999-446049</u>	19991215
<u>US 2002045654</u>	A1	20020418	<u>US 2001-841348</u>	20010424
<u>US 6608095</u>	B2	20030819		
<u>US 2003225064</u>	A1	20031204	<u>US 2003-465767</u>	20030618
<u>US 6727238</u>	B2	20040427		
PRIORITY APPLN. INFO.:			<u>WO 1998-IB912</u>	W 19980611
			<u>WO 1999-IB970</u>	W 19990531
			<u>US 1999-446049</u>	A3 19991215
			<u>US 2001-841348</u>	A3 20010424

OTHER SOURCE(S): MARPAT 132:35714
 GI



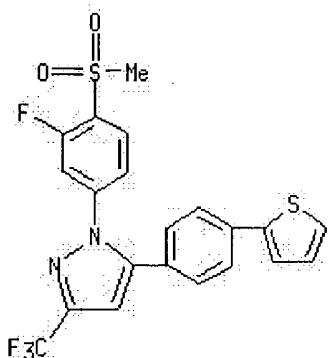
AB This invention provides a compd. of formula (I) or its pharmaceutically acceptable salt thereof [wherein A is partially unsatd. or unsatd. five membered heterocyclic, or partially unsatd. or unsatd. five membered carbocyclic, wherein the 4-(sulfonyl)phenyl and the 4-substituted Ph in formula I are attached to ring atoms of Ring A, which are adjacent to each other; R1 is optionally substituted aryl or heteroaryl, with the proviso that when A is pyrazole, R1 is heteroaryl; R2 is C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkylamino, C1-4 dialkylamino or amino; R3, R4 and R5 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl or the like; or two of R3, R4 and R5 are taken together with atoms to which they are attached and form a 4-7 membered ring; R6 and R7 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, C1-4 alkylamino or N,N-di C1-4 alkylamino; and m and n are independently 1, 2, 3 or 4]. This invention also provides a pharmaceutical compn. useful for the treatment of a medical condition in which prostaglandins are implicated as pathogens. This invention relates to compd. and pharmaceutical compns. for the treatment of cyclooxygenase mediated diseases. These compds. inhibit the biosynthesis of prostaglandins by intervention of the action of the enzyme cyclooxygenase on arachidonic acid, and are therefore useful in the treatment or alleviation of inflammation and other inflammation assocd. disorders, such as arthritis, in mammals (no data). Thus, To a stirred soln. of 1-[4-(Methylsulfonyl)phenyl]-5-(4-bromophenyl)-3-trifluoromethyl-1H-pyrazole (0.27 g) in DME (8 mL) was added 3-thiophenboronic acid (0.09 g), bis(triphenylphosphine)palladium(II)chloride (0.05 g) and satd. NaHCO₃ soln. (2 mL) at room temp. under nitrogen. The mixt. was heated at reflux temp. for 16 h, and cooled down to room temp. to give, after purifn. by flash chromatog. eluting with Et acetate/hexane (1/1), 1-[4-(Methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-trifluoromethyl-1H-pyrazole (II) in 64 % yield.

IT **252559-81-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclyl sulfonylbenzene compds. as cyclooxygenase inhibitors, prostaglandin biosynthesis inhibitors, anti-inflammatory, and analgesic agents)

RN 252559-81-2 HCAPLUS

CN 1H-Pyrazole, 1-[3-fluoro-4-(methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text
References

ACCESSION NUMBER: 1999:82258 HCAPLUS
DOCUMENT NUMBER: 130:210722
TITLE: Synthesis and properties of novel aziridinyl azo dyes from 2-aminothiophenes-Part 2: Application of some disperse dyes to polyester fibers
AUTHOR(S): Hallas, Geoffrey; Choi, Jae-Hong
CORPORATE SOURCE: Dep. Colour Chemistry and Dyeing, Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Dyes and Pigments (1998), Volume Date 1999, 40(2-3), 119-129
CODEN: DYPIDX; ISSN: 0143-7208
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of yellow to greenish-blue aziridinyl azo dyes and their bromoethylamino azo precursors contg. a thienyl coupling moiety has been applied to conventional polyester fiber as well as microdenier polyester by high temp. exhaust dyeing. Heat transferability of these dyes onto polyester fiber has also been examd., using conventional heat-transfer printing techniques. The relevant dyeing characteristics, heat transferability, build-up, dyeability on microfiber polyester, washfastness, and lightfastness are given. These aziridinyl dyes are reactive to polyester fibers under HT dyeing conditions. Fabrics dyed with aziridinyl dyes re more resistant to solvent extn. than those dyed with conventional dyes. Residual liquors showed only a pale color when fabric dyed with aziridinyl dyes was dissolved and then pptd., whereas a colored polyester ppt. was obtained.

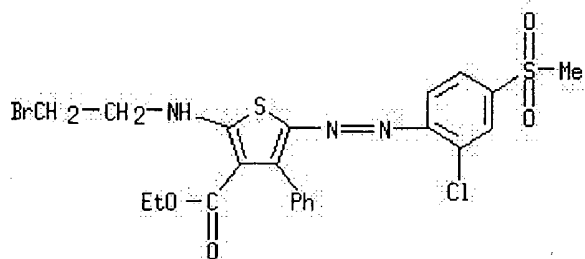
IT 220964-99-8

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(brown dye; fastness to polyester under high-temp. exhaust dyeing and thermal-transfer printing conditions)

RN 220964-99-8 HCAPLUS

CN 3-Thiophenecarboxylic acid, 2-[(2-bromoethyl)amino]-5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER: 1999:82257 HCAPLUS
 DOCUMENT NUMBER: 130:210776
 TITLE: Synthesis and properties of novel aziridinyl azo dyes from 2-aminothiophenes-Part 1: Synthesis and spectral properties
 AUTHOR(S): Hallas, Geoffrey; Choi, Jae-Hong
 CORPORATE SOURCE: Department Colour Chemistry and Dyeing, Univ. Leeds, Leeds, LS2 9JT, UK
 SOURCE: Dyes and Pigments (1998), Volume Date 1999, 40(2-3), 99-117
 CODEN: DYPIDX; ISSN: 0143-7208
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A series of yellow to greenish-blue aziridinyl azo dyes and their bromoethylamino azo precursors contg. a thienyl coupling moiety has been prepd. from 2-aminothiophenes. The 2-aminothiophenes were readily obtained by using the Gewald reaction. It was found that cyclization of the precursor dyes to the corresponding aziridine azo dyes brought about bathochromic shifts in absorption maxima. Further spectral comparisons with N-Ph azo dyes derived from other terminal 4-, 5-, 6-, 7-, and 8-membered cyclic groups showed that the N-thienylaziridinazo dyes are relatively bathochromic. From the viewpoint of solvatochromism, a clear contrast existed between λ_{\max} values in different solvents; thus, a pos. solvatochromism was obsd. in aprotic solvents, whereas a hypsochromic shift was brought about in polar protic solvents. PPP-MO calcns. provided reliable predictions of absorption maxima for the various aziridinyl azo dyes and their precursor dyes.

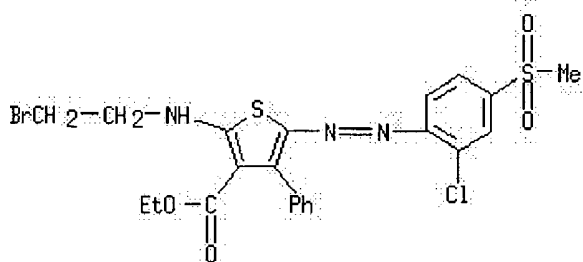
IT 220964-99-8P

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(brown dye intermediate; prepn. of aziridinyl azo dyes from 2-aminothiophene coupling components)

RN 220964-99-8 HCAPLUS

CN 3-Thiophenecarboxylic acid, 2-[(2-bromoethyl)amino]-5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Chang
References

ACCESSION NUMBER: 1997:421308 HCAPLUS
DOCUMENT NUMBER: 127:34521
TITLE: Preparation of hydrazidyl, bis-hydrazidyl, and bis-aminomethyl carbonyl protease inhibitors
INVENTOR(S): Carr, Thomas Joseph; Desjarlais, Renee Louise; Gallagher, Timothy Francis; Halbert, Stacie Marie; Oh, Hye-Ja; Thompson, Scott Kevin; Veber, Daniel Frank; Yamashita, Dennis Shinji; et al.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 253 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9716433	A1	19970509	WO 1996-US18000	19961030
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, US, US, US, US, US, US, US, US, US, US, US, US, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9609078	A	19980429	ZA 1996-9078	19961029
CA 2236111	AA	19970509	CA 1996-2236111	19961030
AU 9711180	A1	19970522	AU 1997-11180	19961030
CN 1207095	A	19990203	CN 1996-199284	19961030
BR 9612344	A	19990713	BR 1996-12344	19961030
EP 934291	A1	19990811	EP 1996-941981	19961030
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO				
NO 9801938	A	19980629	NO 1998-1938	19980429
US 5998470	A	19991207	US 1999-290958	19990413
US 6057362	A	20000502	US 1999-330287	19990611
US 6232342	B1	20010515	US 1999-330451	19990611
US 6284777	B1	20010904	US 2000-552616	20000419
US 6331542	B1	20011218	US 2000-551968	20000419
NO 2000006716	A	19980629	NO 2000-6716	20001229
NO 2000006717	A	19980629	NO 2000-6717	20001229
NO 2000006718	A	19980629	NO 2000-6718	20001229
CN 1341590	A	20020327	CN 2001-104787	20010220
CN 1341592	A	20020327	CN 2001-104788	20010220

CN 1341593	A	20020327	CN 2001-104789	20010220
US 2002077455	A1	20020620	US 2001-839410	20010420
US 6586466	B2	20030701		
US 2002173469	A1	20021121	US 2002-160314	20020530
US 6562842	B2	20030513		

PRIORITY APPLN. INFO.:

US 1995-8108P	P	19951030
US 1995-7473P	P	19951122
US 1995-8992P	P	19951221
US 1996-13747P	P	19960320
US 1996-13748P	P	19960320
US 1996-13764P	P	19960320
US 1996-17455P	P	19960517
US 1996-17892P	P	19960517
US 1996-22047P	P	19960722
US 1996-23494P	P	19960807
WO 1996-US18000	W	19961030
US 1997-793915	A3	19970214
US 1998-793915	B3	19980430
US 1999-330284	B1	19990611
US 1999-330305	B1	19990611
US 2000-633700	B1	20000807

OTHER SOURCE(S): MARPAT 127:34521

AB Title compds. of formula D-CO-Q [D = CbzNHCH(Bu-i), Cbz-Leu-NHCH(Bu-i), 4-PhOC6H4SO2NHCH2, Cbz-Leu-NHNH, etc.; Q = NHCH(Bu-i)(2-carboxythiazol-4-yl), NHCH(Bu-i)(4-carboethoxythiazol-2-yl), NHNHCOCH(Bu-i)NHCbz, CH2NHSO2C6H4-4-OPh, etc.; Cbz = PhCH2O2C] and pharmaceutical compns. of such compds., which inhibit proteases, including cathepsin K (no data) were prepd. Such compds. are particularly useful for treating diseases of excessive bone loss or cartilage or matrix degrdn., e.g. osteoporosis, periodontitis, and arthritis. For example, Cbz-Leu-Leu-CH2Br was treated with H2NCSCO2Et in refluxing ethanol for 4 h to give Cbz-Leu-NHCH(Bu-i)(2-carboethoxythiazol-4-yl), which was sapond. by treatment with sodium hydroxide in THF to yield title compd. Cbz-Leu-NHCH(Bu-i)(2-carboxythiazol-4-yl).

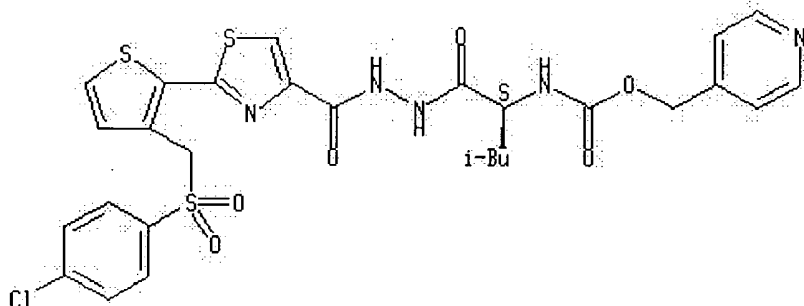
IT 190658-17-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hydrazidyl, bis-hydrazidyl, and bis-aminomethyl carbonyl protease inhibitors)

RN 190658-17-4 HCAPLUS

CN 4-Thiazolecarboxylic acid, 2-[3-[[[(4-chlorophenyl)sulfonyl]methyl]-2-thienyl]-, 2-[(2S)-4-methyl-1-oxo-2-[[[(4-pyridinylmethoxy)carbonyl]amino]pentyl]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

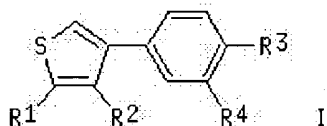


L6 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER: 1995:339482 HCAPLUS
 DOCUMENT NUMBER: 122:105655
 TITLE: Preparation of 2-substituted-3,4-di(aryl)thiophene
 cyclooxygenase inhibitors
 INVENTOR(S): Gauthier, Jacques Yves; Leblanc, Yves; Prasit,
 Petpiboon
 PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.
 SOURCE: PCT Int. Appl., 42 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9426731	A1	19941124	WO 1994-CA264	19940511
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TT, UA, US, UZ RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2161789	AA	19941124	CA 1994-2161789	19940511
AU 9467184	A1	19941212	AU 1994-67184	19940511
PRIORITY APPLN. INFO.:				
			US 1993-61354	A 19930513
			WO 1994-CA264	W 19940511
OTHER SOURCE(S): MARPAT 122:105655				
GI				



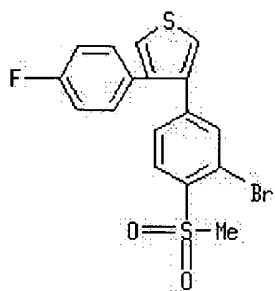
AB The title compds. [I; R1 = H, halogen, CN, NO2, CF3, C1-6 alkyl; R2 = C3-6
 alkyl, (un)substituted Ph, (un)substituted heteroaryl; R3 = SO2CH3,
 S(O)(NH)CH3, SONH2, SO2NH2; R4 = H, halogen, CO2H, CF3], useful as
 cyclooxygenase inhibitors, are prepd. and I-contg. formulations claimed.
 Thus, 3-(4-fluorophenyl)-4-(4-sulfamoylphenyl)thiophene was prepd. and
 demonstrated 95% inhibition of PGE2 formation by osteosarcoma (143.98.2)
 cells at 100 nM.

IT 160753-08-2

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (prepn. of 2-substituted-3,4-di(aryl)thiophene cyclooxygenase
 inhibitors)

RN 160753-08-2 HCAPLUS

CN Thiophene, 3-[3-bromo-4-(methylsulfonyl)phenyl]-4-(4-fluorophenyl)- (9CI)
 (CA INDEX NAME)

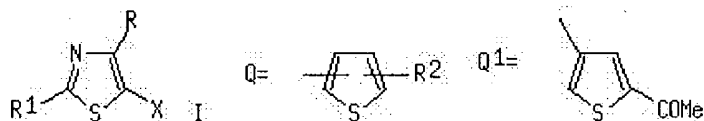


L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Cited References
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ACCESSION NUMBER: 1987:5016 HCAPLUS
 DOCUMENT NUMBER: 106:5016
 TITLE: Thiazolylthiophene derivatives
 INVENTOR(S): Saeki, Sumi; Kawakita, Takeshi; Moriguchi, Akihiko; Osuga, Kunio
 PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61118383	A2	19860605	JP 1984-237865	19841112
PRIORITY APPLN. INFO.:			JP 1984-237865	19841112
OTHER SOURCE(S):		CASREACT 106:5016		
GI				



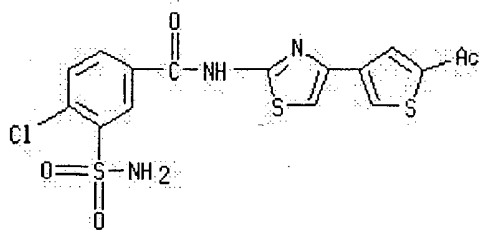
AB The title compds. [I; R = Q; R1 = (substituted) amino; R2 = alkanoyl, CH₂COR₃ (R₃ = OH, alkoxy, substituted amino), X = H, halo], useful as antiulcer agents, etc. (no data), were prepd. Thus, cyclocondensation of Q1COCH₂Cl with (H₂N)₂CS in EtOH at 50° and acylation of the resulting I (R = Q1; R1 = NH₂) with pivaloyl chloride in pyridine gave I (R = Q1; R1 = pivalamido).

IT 105652-30-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as antiulcer agent)

RN 105652-30-0 HCAPLUS

CN Benzamide, N-[4-(5-acetyl-3-thienyl)-2-thiazolyl]-3-(aminosulfonyl)-4-chloro- (9CI) (CA INDEX NAME)



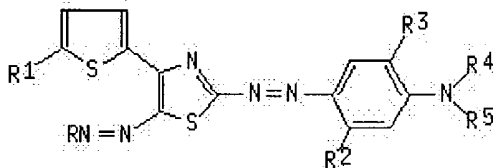
L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
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ACCESSION NUMBER: 1983:145034 HCAPLUS
 DOCUMENT NUMBER: 98:145034
 TITLE: Thienylthiazole disazo disperse dyes
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57177060	A2	19821030	JP 1981-62070	19810424
JP 01034266	B4	19890718		
GB 2101623	A	19830119	GB 1982-11221	19820419
GB 2101623	B2	19840822		
DE 3215123	A1	19821209	DE 1982-3215123	19820423
DE 3215123	C2	19900308		
CH 647537	A	19850131	CH 1982-2539	19820426
US 4841036	A	19890620	US 1984-683323	19841218
PRIORITY APPLN. INFO.:			JP 1981-62070	19810424
			US 1982-372264	19820426

GI



I

AB I (R = Ph, pyridyl, thiazolyl; R1 = H, Cl, Br, Ac; R2 = H, Cl, Br, Me, acylamino; R3 = H, Cl, Me, MeO, EtO; R4, R5 = H, alkyl, cyclohexyl, alkenyl, aryl) were prepd. and were used for dyeing polyester fibers in fast navy blue to green shades. I showed excellent stability to temp. and pH changes during dyeing. For example, aniline [62-53-3] was diazotized and coupled with 2-amino-4-(2-thienyl)thiazole [28989-50-6], and the 2-amino-5-(phenylazo)-4-(2-thienyl)thiazole [85242-87-1] obtained was diazotized and coupled with N-(2-acetoxyethyl)-N-ethylaniline [38954-40-4] to give I (R = Ph; R1 = R2 = R3 = H; R4 = Et; R5 = CH2CH2OAc) [85242-88-2], navy blue on polyester fiber.

IT 85242-65-5

RL: TEM (Technical or engineered material use); USES (Uses)
 (dye, for polyester fibers)

RN 85242-65-5 HCAPLUS

h

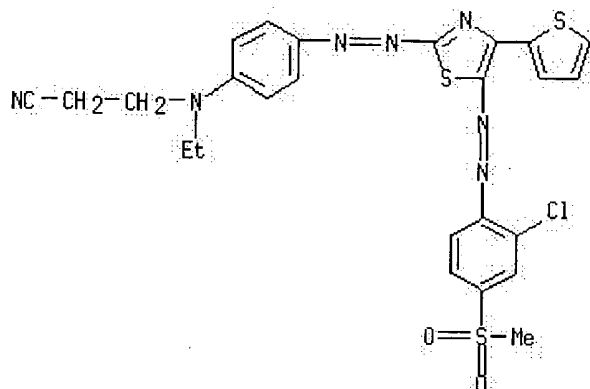
eb c

g cg b

cg

eb

CN Propanenitrile, 3-[[4-[[5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-(2-thienyl)-2-thiazolyl]azo]phenyl]ethylamino]- (9CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
74.92	231.81

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
-10.29	-10.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter [HELP FIRST](#) for more information.

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FILE 'REGISTRY' ENTERED AT 10:54:48 ON 09 AUG 2004

L1 STRUCTURE UPLOADED
L2 2 S L1
L3 41 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 10:57:16 ON 09 AUG 2004

L4 14 S L3
L5 2 S L4 AND BROWN, D?/AU

L6 12 S L4 NOT L5
L7 0 S L6 AND GRANETO, M?/AU
L8 0 S L6 AND LUDWIG, C?/AU

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L9 0 L3

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